

FIG. 2

ATOM TYPES

| | | | |
|-------|---|--------------------|----------|
| C.3 | sp ³ carbon | H | hydrogen |
| C.2 | sp ² carbon | F | fluorine |
| C.1 | sp ¹ carbon | CL | chlorine |
| C.ar | aromatic carbon | BR | bromine |
| C.cat | cationic carbon | I | iodine |
| N.3 | sp ³ nitrogen | | |
| N.2 | sp ² nitrogen | <u>Group Types</u> | |
| N.1 | sp ¹ nitrogen | NO ₂ | |
| N.ar | aromatic nitrogen | NO | |
| N.am | amide nitrogen | CN | |
| N.pl3 | planar sp ³ nitrogen | CO | |
| N.4 | protonated sp ³ nitrogen | SO ₂ | |
| O.3 | sp ³ oxygen | SO | |
| O.2 | sp ² oxygen | OH | |
| O.CO2 | oxygen in carboxylate and phosphate groups | | |
| S.3 | sp ³ sulfur | | |
| S.2 | sp ² sulfur | | |
| S.O | sulfoxide sulfur | | |
| S.O2 | sulfone sulfur | | |
| P.3 | sp ³ phosphorous | | |

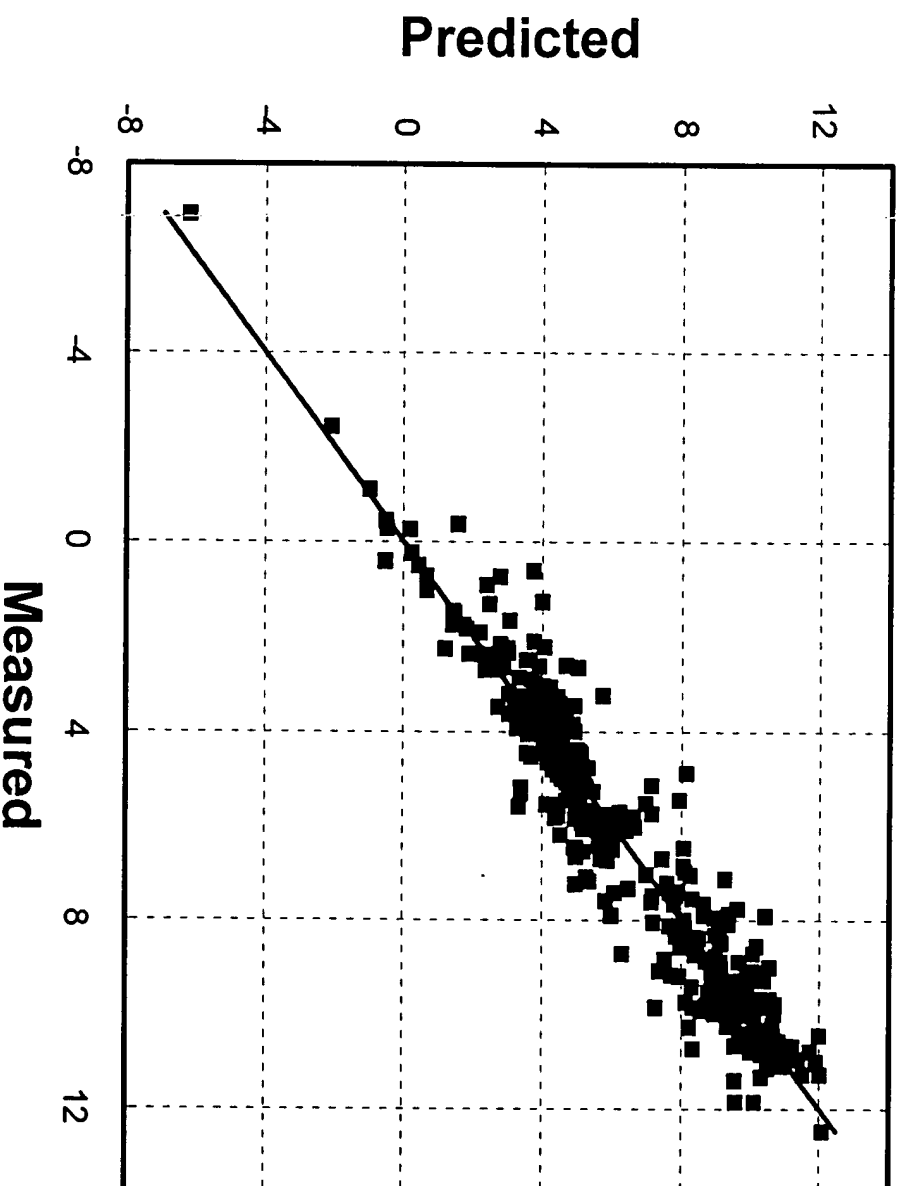
N.ar C.ar H N.pl3

[illegible]

Construction of the hierarchical tree from one example, 6-amino quinoline

pK_a of Bases (384)

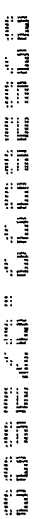
PC = 5, $r^2=0.922$ $q^2=0.832$, Std. Err = 0.89



F15.7

Table 1. Mean values of the variables measured during the 60-min test

PC = 6, $r^2 = 0.927$, $q^2 = 0.792$, Std. Err = 0.77

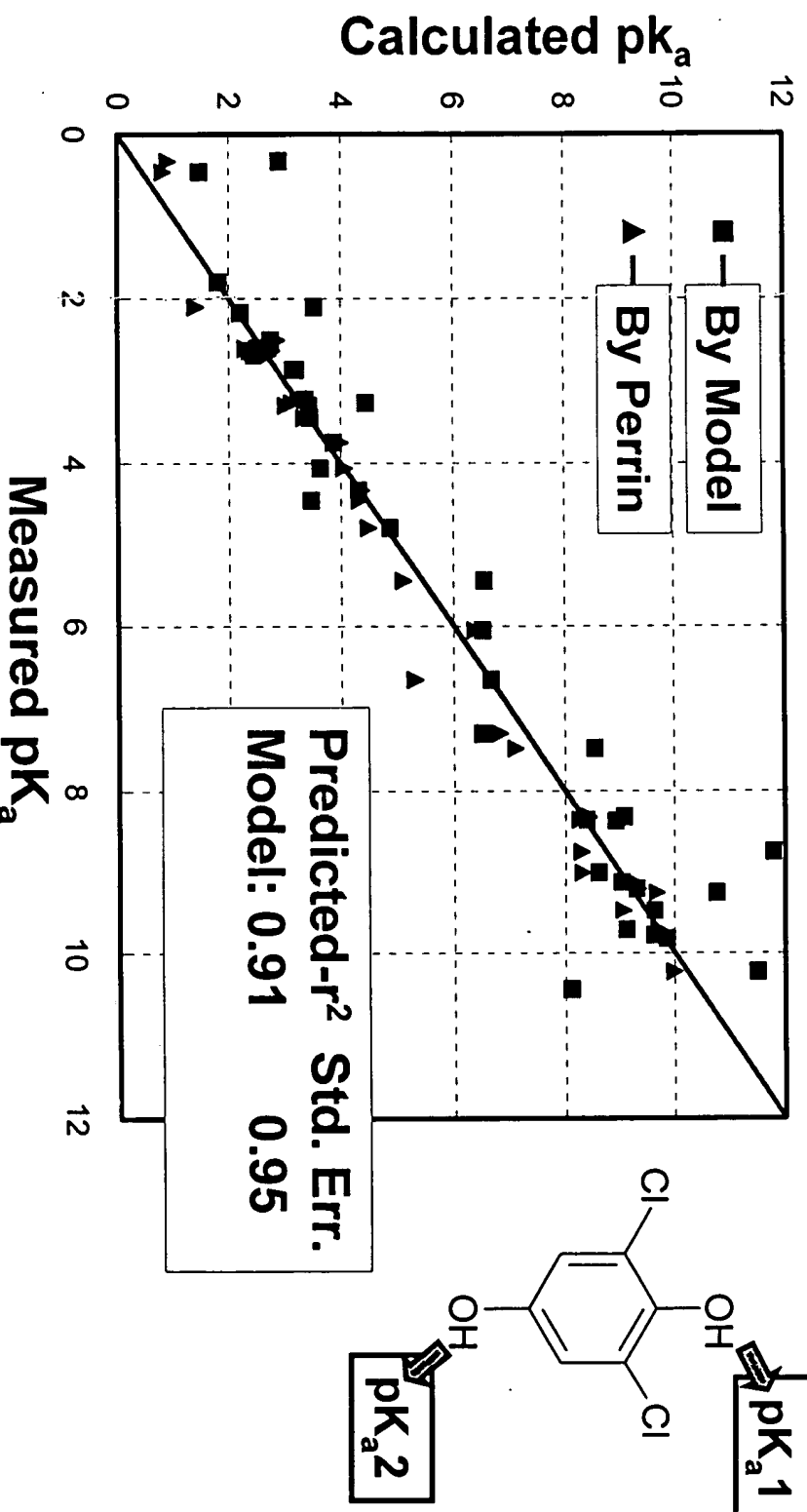


F15.8

Prediction on Molecules

37 acid and base molecules selected by Perrin* *et al.* as examples, and were not included in the training set

For molecules containing multiple ionizable centers the model correctly predicted the order for all of them, ie



*Perrin DD, Dempsey B, Sericant EP, *pKa prediction for organic acids and bases*, Chapman and Hall, London, 1981.